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Numerical analysis of methane ignition phenomenon under Mild Combustion condition

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Abstract

This work presents the results of a modeling study of the ignition process of methane under Mild Combustion conditions. A mathematical model was formulated to predict the dependence of the equivalence ratio Φ and the initial temperature of oxidizer t on the temperature increment $\Delta T = t_{\max} - t$. The increment of temperature was assumed as parameter characterizing the process of ignition. The model incorporates the basic principles of the energy and mass balance. The results of calculation were compared with the experiments which have been done on constant volume bomb (CVB) reactor. It is shown that in order to achieve the effective reaction of ignition it is not necessary to maximize the initial oxidizer temperature. There are optimal values of temperature oxidizer ($t \approx 830^\circ\text{C}$) in which parameters mentioned above reaches its extreme values.

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1. Introduction

Ignition, which is one of the most important parts of combustion and directly affects combustion efficiency and emission, has been the subject of many studies that try to elucidate the ignition characteristic. Excellent description of ignition phenomenon can be found in [1], however, ignition in general is an enormous subject, and the present work cannot provide a thorough treatment. In this paper, the ignition process of methane under Mild Combustion conditions is analysed. Previously, many of the characteristics of Mild Combustion have been investigated in laboratory-scale systems, but the knowledge of both experimental and numerical studies of the gaseous fuel ignition phenomenon under high temperature is an example of the gap in the research of this technology. The Leeds methane oxidation

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mechanism was used to run the model. This mechanism considered 35 reactive species and 190 reactions. Chemkin software was used for combustion simulations with detailed chemistry.

2. Materials and methods

In the present work, time-dependent computations were done assuming laminar flow. Thus, the turbulent mixing and associated effects on chemical reactions were not considered. Presented computations model was limited to the onset of the ignition. The system (a closed constant volume vessel containing a given mass m such that the density $\rho=m/V$ remains constant during the ignition process) is analyzed “after loaded”. The cold fuel was injected into the vessel filled initially with hot air at atmospheric pressure. Heat transfer to the chamber walls is analyzed (combustion chamber was not assumed to be adiabatic). Gases are treated as ideal gases, the governing equations concerns the gaseous combustible mixture. The transient state is taken into consideration. Gravitational acceleration and viscous dissipation were neglected. The governing equations consisted of the mixture mass continuity equation, energy equation and Gibbs function equation. The equations were presented earlier [2].

3. Result and discussion

An example of the determination of the increment of temperature ΔT is presented in Figure 1 [3]. Point “0” is interpreted as the moment of the gas injection and the start of ignition.

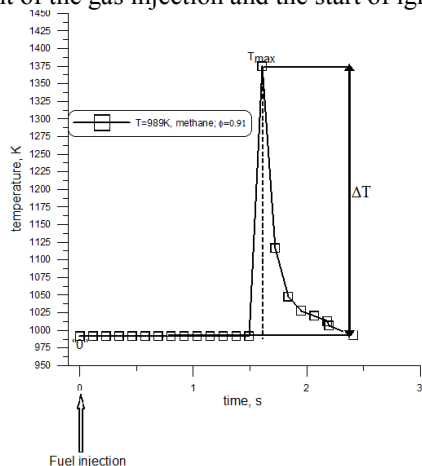


Figure 1. Example of the increment of the temperature ΔT as a function of the duration of the test

The temperature distance between point “0” and the point in which the temperature reaches its maximum is determined as the increment of temperature ΔT . Experimental tests were performed on the special CVB stand (Fig. 2), which has been described before [4]. Next Figure illustrates the dependence of the increment of temperature ΔT as a function of the equivalence ratio at the oxidizer temperature equal 716, 831 and 961°C (Fig. 3a) and as a function of oxidizer temperature for equivalence ratio equal 0.50, 0.91 and 1.43 (Fig 3b). It can be observed for each test, initially the increment of temperature ΔT increases at the beginning with a growth of oxidizer temperature t . It is connected with the relationship that with the growth of the oxidizer temperature t , the reaction rate and frequency of particle collision are both increasing. There is value of oxidizer temperature t in which the increment of temperature ΔT reaches its maximum. The highest values of ΔT are achieved for $t=831^{\circ}\text{C}$. Above the value of t in which the increment ΔT reaches its maximum (ΔT_{max}), this parameter is decreasing due to smaller level of density

(concentration) of reacting gases at constant pressure (chamber is not hermetic). It can be concluded that despite the fact that increment of oxidizer temperature ΔT favours growth of reaction rate, the decrease of gas density is much stronger. As a result, above the value of it, in which $\Delta T = \Delta T_{\max}$, this parameter is decreased. It seems that preheating oxidizer above this value of temperature oxidizer, which equals approximately $t \approx 830^\circ\text{C}$, is unsubstantiated. Similar diagrams have been plotted for all analyzed values of equivalence ratio, but it is well known that most combustion properties have simple maxima or minima in the neighbourhood of $\phi = 1$. It is worthwhile to emphasize one important feature. Methane as majority of alkanes inhibits its own ignition [5] when the rate of branching of chain branching (as an essential reaction for the high temperature combustion) is higher than the rate of tearing off of chain branching. Hydrogen atoms and alkyl radicals (the most important products of chain branching) in different conditions are characterized by different properties. It can be noticed that for rich mixtures ($\phi > 1$) alkanes are inhibitors of ignition reaction due to the important rerouting of hydrogen atoms from chain branching reaction. This feature is predominating over ignition so increment temperature decreases with the growth of ϕ . For lean mixtures ($\phi < 1$), not very often collisions between oxidizing and reducing species (small presence of fuel) are limiting the rerouting of hydrogen atoms (favourable factor). Here, alkanes behave like promoters of their own ignition. In this case, increment temperature increases with the growth of ϕ . For values ϕ in which ΔT reaches its maximum, there is a balance between the amount of reactive radicals and not very well reactive hydrogen atoms.

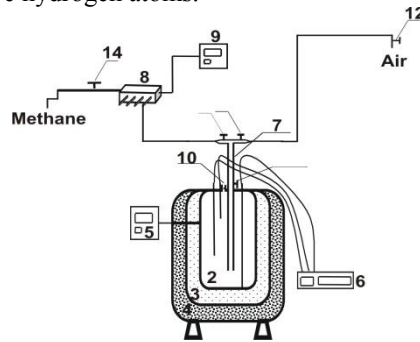


Figure 2. Scheme of the constant volume bomb (CVB); 1, reaction chamber, 2, heating coil, 3, thermal insulation, 4, microprocessor control unit, 5, digital recorder, 6, conduit supplying gas, 7, electric valve, 8, control unit, 9, safety vent, 10-13, valves

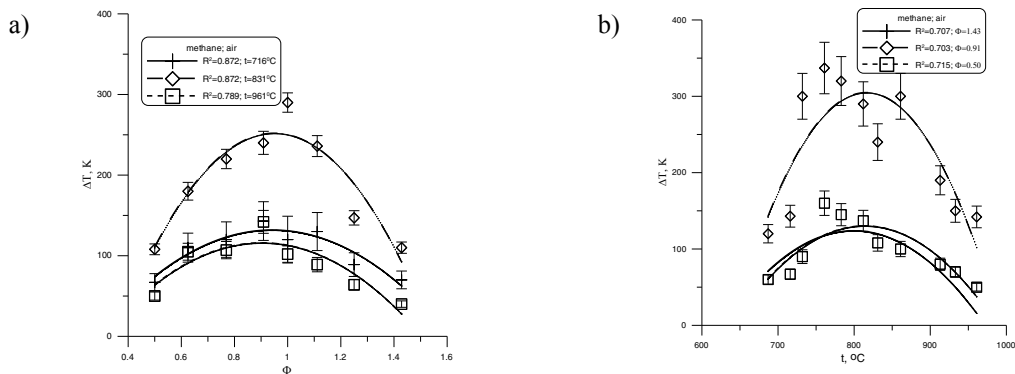


Figure 3. Dependence of the increment of temperature as a function of equivalence ratio (a) and temperature of the oxidizer (b); results of experiment

Comparison of experimental results with numerical simulations

Figures 4 a and b show the measured and calculated increment temperatures using Leeds Methane oxidation Mechanism. As can be seen, the calculation using the Leeds Mechanism shows good agreement with the measurements over the range of oxidizer temperature and equivalence ratio studied.

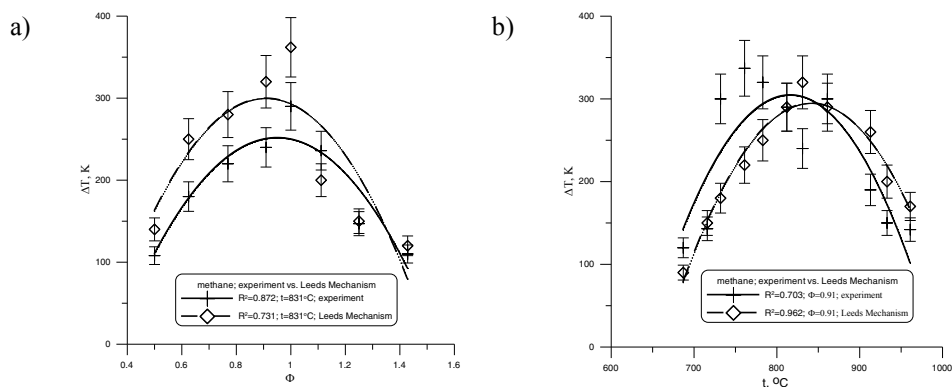


Figure 4. The dependence of the increment of temperature as a function of equivalence ratio (a) and oxidizer temperature (b); comparison of the experiment results and calculation using Leeds Mechanism

4. Conclusions

In this work the ignition of methane was investigated with the use of different high temperature oxidizers. Moreover, a constant volume bomb (CVB) was applied in the investigation. Taking into consideration analyzed parameter (ΔT), it seems that preheating the oxidizer without limits seems to be unsubstantiated. There is the value of temperature oxidizer ($t \approx 830$ °C) in which analyzed parameter reaches its extreme values. Very good agreement between the measurements and calculations using Leeds Mechanism of methane oxidation is observed. Over the entire operating range of temperatures of oxidizer and equivalence ratio used in the present study, the differences between the measured and calculated values of the increment temperature are less than 25%.

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